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REPORT NO. 1433

RESOLUTION OF STRESSES IN DEFORMATION TWINNING

by

Priscilla W. Kingman

April 1969

JUL 7 1969

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ABERDEEN PROVING GROUND, MARYLAND

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Terminal Ballistics Laboratory

ABERDEEN PROVING GROUND, MARYLAND

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PWKingman/thg
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RESOLUTION OF STRESSES IN DEFORMATION TWINNING

ABSTRACT

Solutions for the maximum resolved shear stresses on twinning
systems in fcc and bcc crystals in tension and compression are presented
and discussed. Additional data are included on the relative magnitudes
of shear stresses on secondary systems. Conventions for the specifica-
tion of twinning systems are described and discussed.

TABLE OF CONTENTS

LIST OF SYMBOLS

bcc   body centered cubic lattice

d   specimen diameter

fcc   face centered cubic lattice

ℓ fraction of specimen length transformed in twinning

K_1 first undistorted plane (twin habit plane)

L   initial specimen length

η_1 first undistorted direction (twin shear direction)

λ angle between stress axis and the shear direction

ϕ angle between stress axis and the normal to a shear plane

( )   Miller indices of a plane

[ ]   Miller indices of a direction

{ }   Miller indices of a form

< >   Miller indices of the directions of a form

INTRODUCTION

The deformation twinning of face-centered cubic metals has been the subject of a number of recent investigations. Several authors have discussed the resolution of shearing stresses on twin systems for various orientations;[1,2,3*] unfortunately however, the solutions presented in the literature have been incomplete or incorrect. It therefore appeared desirable to derive a complete solution for the operative systems in tension and in compression and their resolved shear stress factors. Because of the symmetry between the twinning modes of fcc and bcc crystals, the results are easily extended to the bcc case. A systematic tabulation for all four cases is presented below. The results for tensile twinning in bcc crystals are in agreement with those of Allen et al;[4] the remaining cases have not previously been completely given in the literature.

RESULTS

Face centered cubic crystals twin according to the mode {111} <$\bar{2}$11>; because of the polar nature of the <211> axes there are twelve crystallographically equivalent but physical distinct possible twinning systems. Body centered cubic crystals twin according to the mode {$\bar{2}$11} <$\bar{1}\bar{1}\bar{1}$>, thus for each fcc twin system there is a formally related bcc system. Table I contains a listing of the twelve systems for each lattice, along with identifying numbers which refer to Figures 1a and 1b. The choice of indices to specify a given system and the relationship between the bcc and fcc systems bearing the same number will be further discussed in the next section.

The most favored twin systems as a function of specimen orientation are shown in Figures 1a and 1b. The most favored system is taken to be that glide system on which the resolved shear stress resulting from a uniaxial stress along the specimen axis is the greatest. Since the twinning shear is polar, the most favored system in tension and in compression

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References are listed on page 25.

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Table I. Tabulation of Twin Systems

FCC		M	BCC	
K_1	η_1		K_1	η_1
$(1\bar{1}1)$	$[1\bar{1}\bar{2}]$	1	$(\bar{1}12)$	$[1\bar{1}1]$
$(\bar{1}\bar{1}1)$	$[\bar{1}\bar{1}\bar{2}]$	2	(112)	$[\bar{1}\bar{1}1]$
(111)	$[\bar{2}11]$	3	$(\bar{2}11)$	$[\bar{1}\bar{1}\bar{1}]$
$(\bar{1}11)$	$[211]$	4	(211)	$[1\bar{1}\bar{1}]$
$(\bar{1}\bar{1}1)$	$[\bar{1}21]$	5	$(\bar{1}21)$	$[11\bar{1}]$
$(1\bar{1}1)$	$[121]$	6	(121)	$[\bar{1}1\bar{1}]$
(111)	$[11\bar{2}]$	7	$(\bar{1}\bar{1}2)$	$[111]$
$(\bar{1}11)$	$[\bar{1}1\bar{2}]$	8	$(1\bar{1}2)$	$[\bar{1}11]$
$(1\bar{1}1)$	$[\bar{2}\bar{1}1]$	9	$(\bar{2}\bar{1}1)$	$[\bar{1}1\bar{1}]$
$(\bar{1}\bar{1}1)$	$[2\bar{1}1]$	10	$(2\bar{1}1)$	$[11\bar{1}]$
$(\bar{1}11)$	$[\bar{1}\bar{2}1]$	11	$(\bar{1}\bar{2}1)$	$[1\bar{1}\bar{1}]$
(111)	$[1\bar{2}1]$	12	$(1\bar{2}1)$	$[\bar{1}\bar{1}\bar{1}]$

Tabulation of (K_1) (twinning plane) and $[\eta_1]$ (twinning direction) for twin systems in fcc and bcc crystals.
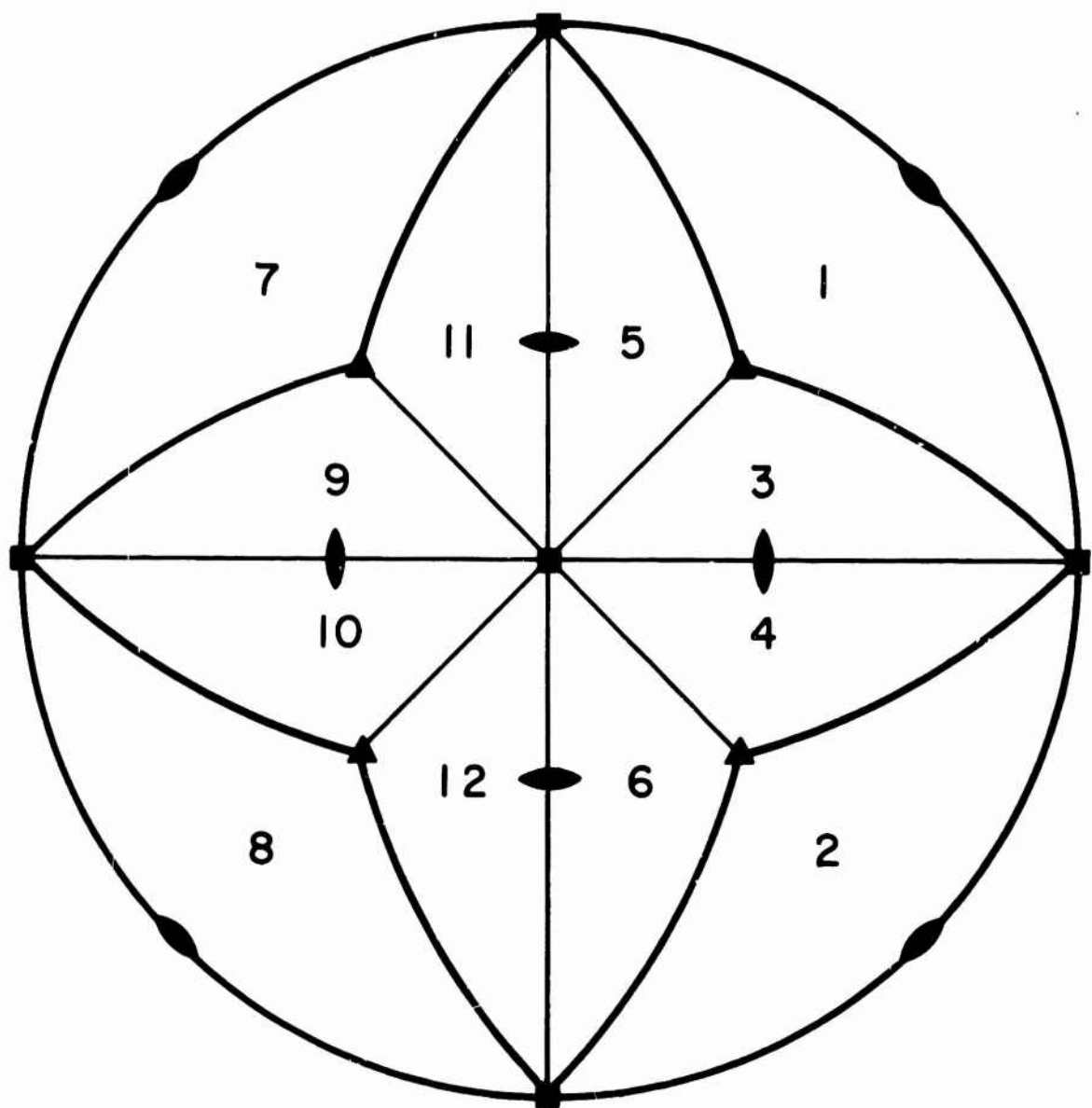
Figure 1a. Twin systems having maximum resolved shear stress as a function of specimen orientation: fcc tension and bcc compression.
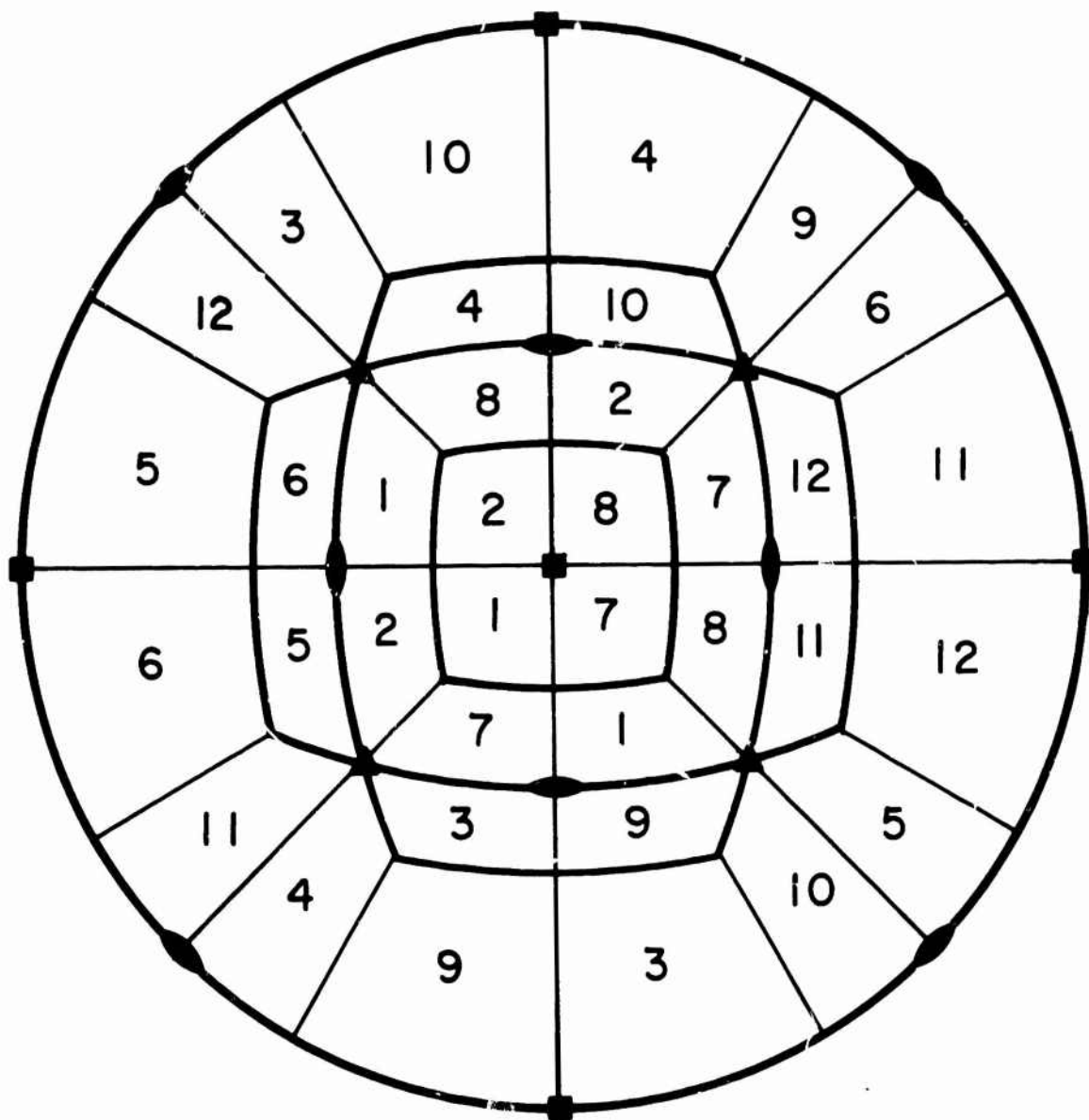
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Figure lb. Twin systems having maximum resolved shear stress as a function of specimen orientation: fcc compression and bcc tension.

will not be the same for a given specimen orientation; the two cases must be considered separately with proper regard for the sign of the applied force. (That the sign of the resolved shear stress rather than the change of length of the specimen axis is the appropriate criterion for the initiation of twinning was shown by Frank and Thompson[5] on the basis of the net work performed by the applied stress during the initiation of a lamellar twin. Actually, the term lamellar is unnecessarily restrictive, since the argument rests on the geometry of shear deformation. When specimens undergo homogeneous shear the original material axis is rotated relative to the stress axis. For the specimen orientations discussed by Frank and Thompson, compressive twinning results in an elongation of the material axis, but because of the accompanying rotation, the dimension normal to the platens becomes smaller and this effect is independent of the width of the twin band. If the specimen geometry is chosen to avoid instability, the only limitation is the intersecion of the twin plane with the ends of the specimen. The fraction of the original specimen length which may be transformed by twinning is thus $\ell = L - d \tan \phi$, where L is the total specimen length, d is the specimen diameter, and ϕ is the angle between K_1 and the specimen axis. Since ϕ is required to be relatively small, it is theoretically possible in many cases to twin a substantial portion of the crystal provided that stability and grip effects are favorable.)

Figure 1a describes either fcc crystals in tension or bcc crystals in compression; the crystallographic specification of the twin system corresponding to a given number is that listed in the column for the appropriate lattice in Table I. Figure 1b represents fcc crystals in compression and bcc crystals in tension. At high symmetry points and along symmetry lines the most favored systems in the adjoining regions are equally favored. Within the standard stereographic triangle, the resolved shear stress on the most favored system varies as a function of $\cos \phi \cos \lambda$ (Schmid factor). Contours of this product for the tension and compression cases are plotted in Figures 2a and 2b. A single plot suffices since the two standard triangles in which each system is favored
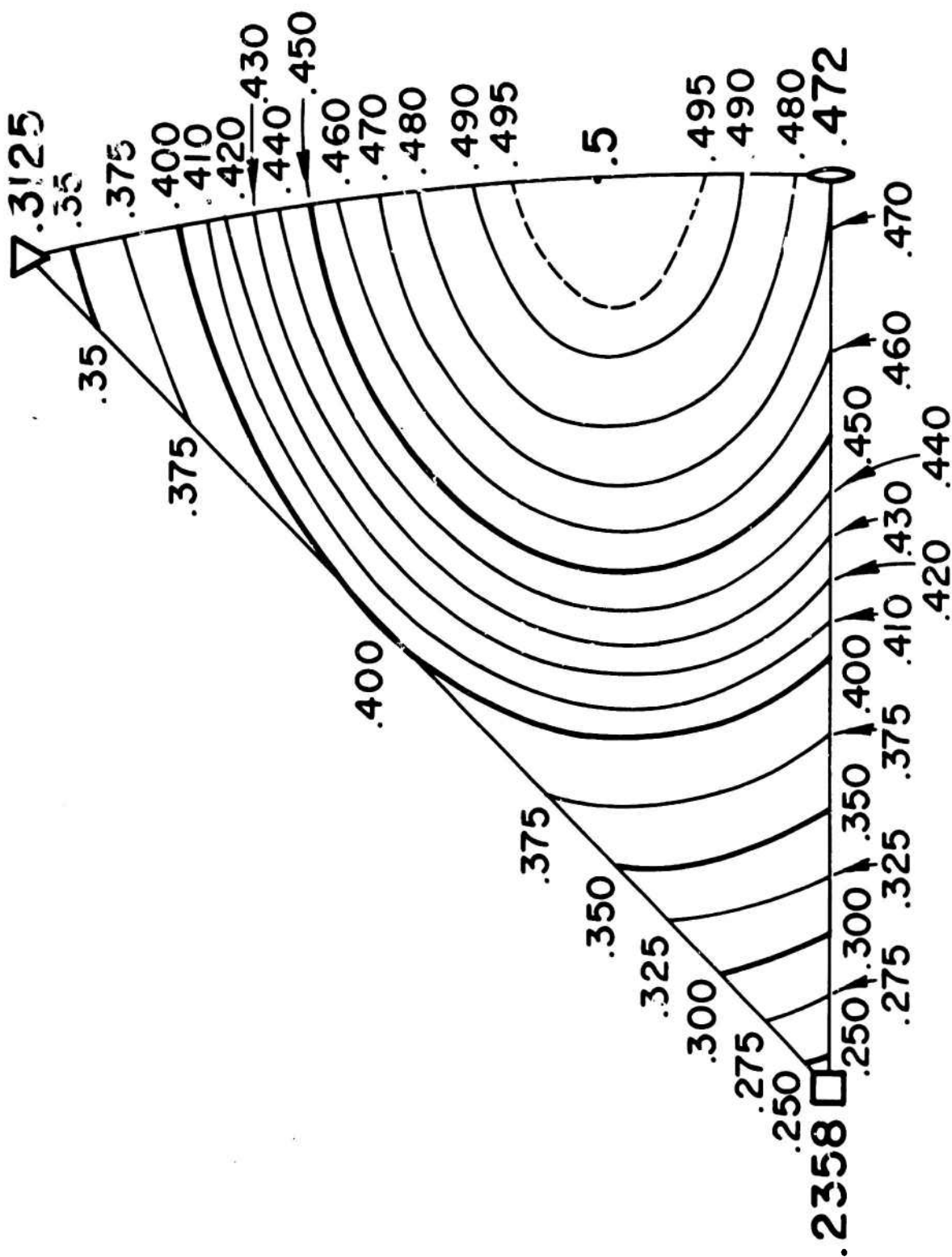
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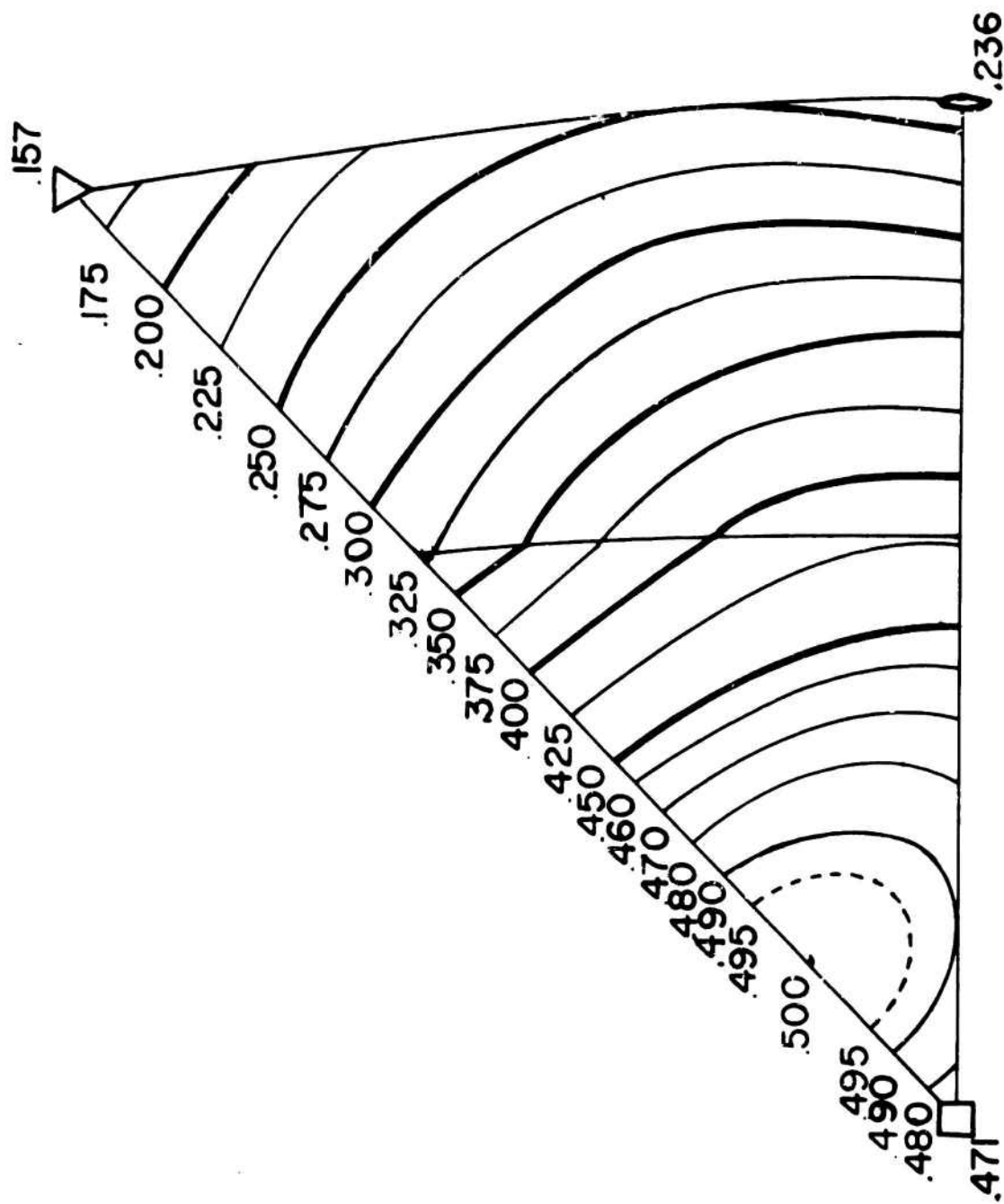Figure 2a. Contours of cos ϕ cos λ as a function of orientation: fcc tension and bcc compression.

Figure 2b. Contours of cos φ cos λ as a function of orientation: fcc compression and bcc tension.

are mirror images of one another. Data for these plots was obtained by
computation over a 2° mesh performed on the Ballistic Research Laboratories
Electronic Scientific Computer (BRLESC).

DISCUSSION

Several aspects of the above solution deserve comment. A continuing
source of confusion in the discussion of twinning in high-symmetry
crystals is the proper enumeration and specification of the crystallo-
graphically equivalent but physically distinct twinning systems $\{K_1\}$ $<n_1>$.
The existence of only twelve physically distinct twinning systems (in
contrast with the twenty-four possible for slip) is a result of the polar
character of the atomic displacements which occur in twinning. Proper
specification of the sense of shear is therefore essential. Since a
plane may be specified by the crystallographic indices of either of its
normals, a single physical twinning shear may be crystallographically
described by either of two alternative sets of indices; for example,
(111) $[\bar{2}11]$ and $(\bar{1}\bar{1}\bar{1})$ $[2\bar{1}\bar{1}]$. In this work it was found most convenient
to choose all $[K_1]$ to lie on the positive side of (001) and the indices
listed in Table I are based upon this convention.

In plotting stereograms of multiple twinning systems, it is advan-
tageous to adopt a convention in which all $[K_1]$'s are chosen to lie on
one side of the plane normal to the stress axis, for in any stereogram
in which the stress axis is plotted at the center and all $[K_1]$'s are
chosen to lie in the upper hemisphere, properly specified $[n_1]$'s will be
activated in tension or in compression accordingly as they fall in the
upper or lower hemispheres. Such a plot is particularly convenient for
specimen axes parallel to high symmetry directions, for it reveals by
inspection the systems activated in tension and compression, which sys-
tems are equally stressed, and the relative magnitudes of their resolved
shear stresses. For example, in Figure 3 a stereogram for a $[001]$ stress
axis shows eight equally stressed systems in tension and four equally
stressed systems in compression, while for a $[111]$ stress axis there are
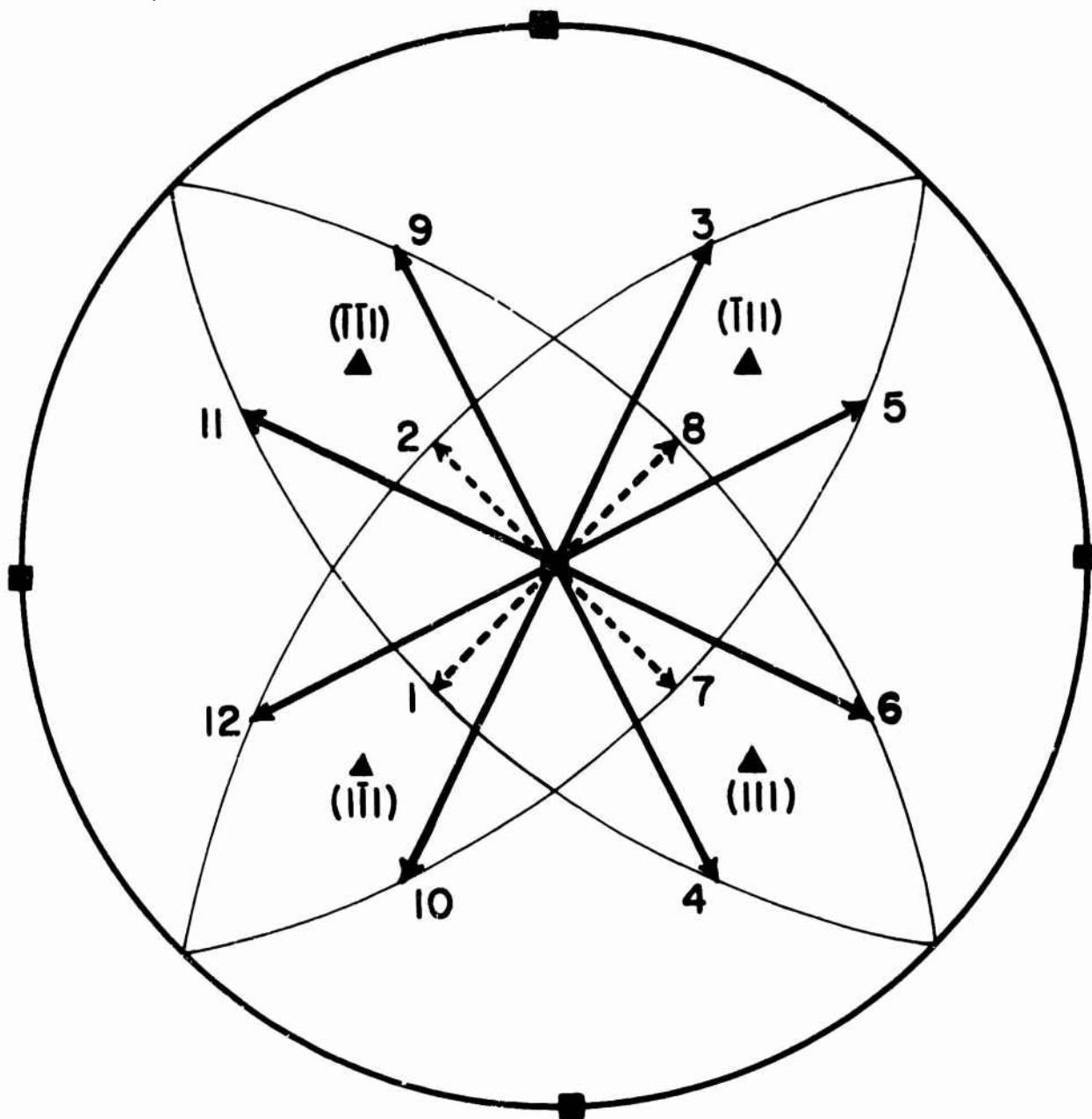three equally stressed systems in tension, six equally stressed systems

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Figure 3a. Stereogram of fcc twin directions $[n_1]$ relative to specimen axes along high symmetry directions, specimen axis [001].
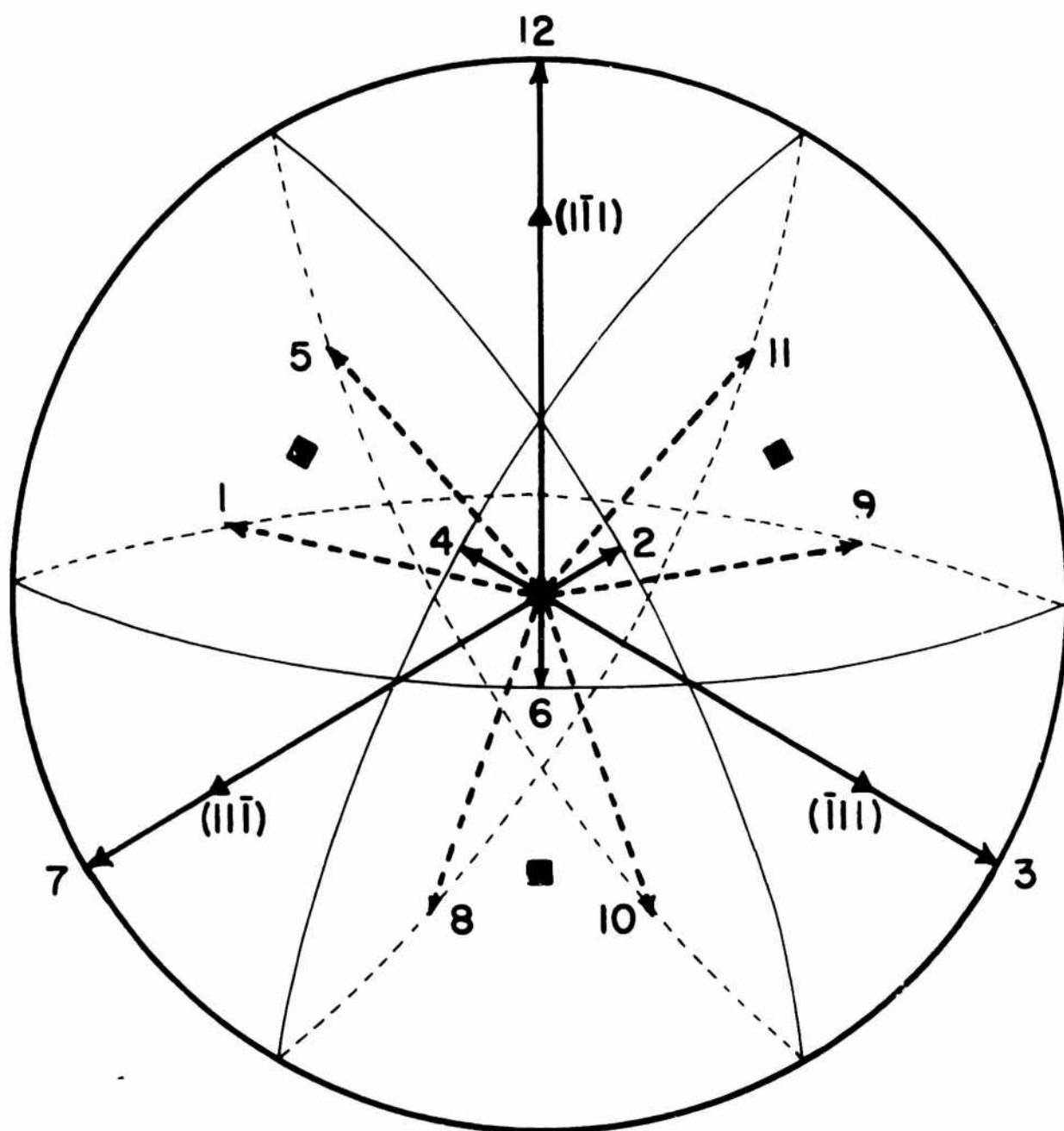
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Figure 3b. Stereogram of fcc twin directions $[\eta_1]$ relative to specimen axes along high symmetry directions, specimen axis [111].

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in compression, and three systems having zero resolved shear stress. In the latter case, note that $[\bar{1}\bar{1}1]$ now lies in the lower hemisphere, so $[11\bar{1}]$ is chosen as $[K_1]$ and systems 2, 5, and 10 are now represented by $(\bar{K}_1)$ $[\bar{n}_1]$ relative to Table 1.

In view of the fact that the crystallography of twinning in fcc and bcc crystals is entirely different -- fcc crystals twin on four octahedral planes while bcc crystals twin on twelve tristetrahedral planes -- it seems surprising at first that the stress resolution should be formally identical except for a change of sign. Part of the symmetry results from the obvious fact that the twin direction of one system is normal to the twin plane of the other; thus regardless of the sense of the twin direction, in computing the resolved shear stress the pair of cosines will have the same magnitude, and the numerical value of the product $\cos \lambda$ $\cos \phi$ will be the same in both cases. Polarity of the twinning shear, however, requires that the sense of the external force -- and hence the sign of the cosine product -- be opposite for the two lattices. This can be easily seen in Figure 4 where the shearing stresses on an element undergoing twinning shear are illustrated for the (111) $[\bar{2}11]$ fcc twin and the $(\bar{2}11)$ $[\bar{1}\bar{1}1]$ bcc twin. The required shears are immediately seen to be opposite in sense for the two cases.

The presence of a symmetry line along the trace of (021) in Figure 1b, dividing the standard triangle into two regions where different systems are favored, should be noted. It has sometimes been implicitly assumed that if one system is most favored at all three corners of the standard triangle, it will be most favored at all points within the triangle.[1,2,3] This condition is in fact necessary but not sufficient, since three special solutions are not necessarily sufficient for the specification of a general solution. Frank and Thompson[5] have elegantly discussed the description of loci where pairs of twin systems are equally favored; the relation between systems 7 and 8, etc., corresponds to their "meta" case. (This locus is given by Allen et al[4] in their thorough treatment of the bcc tension case, but its existence in the fcc compression case appears to have been overlooked despite the symmetrical relationship of the two situations.)
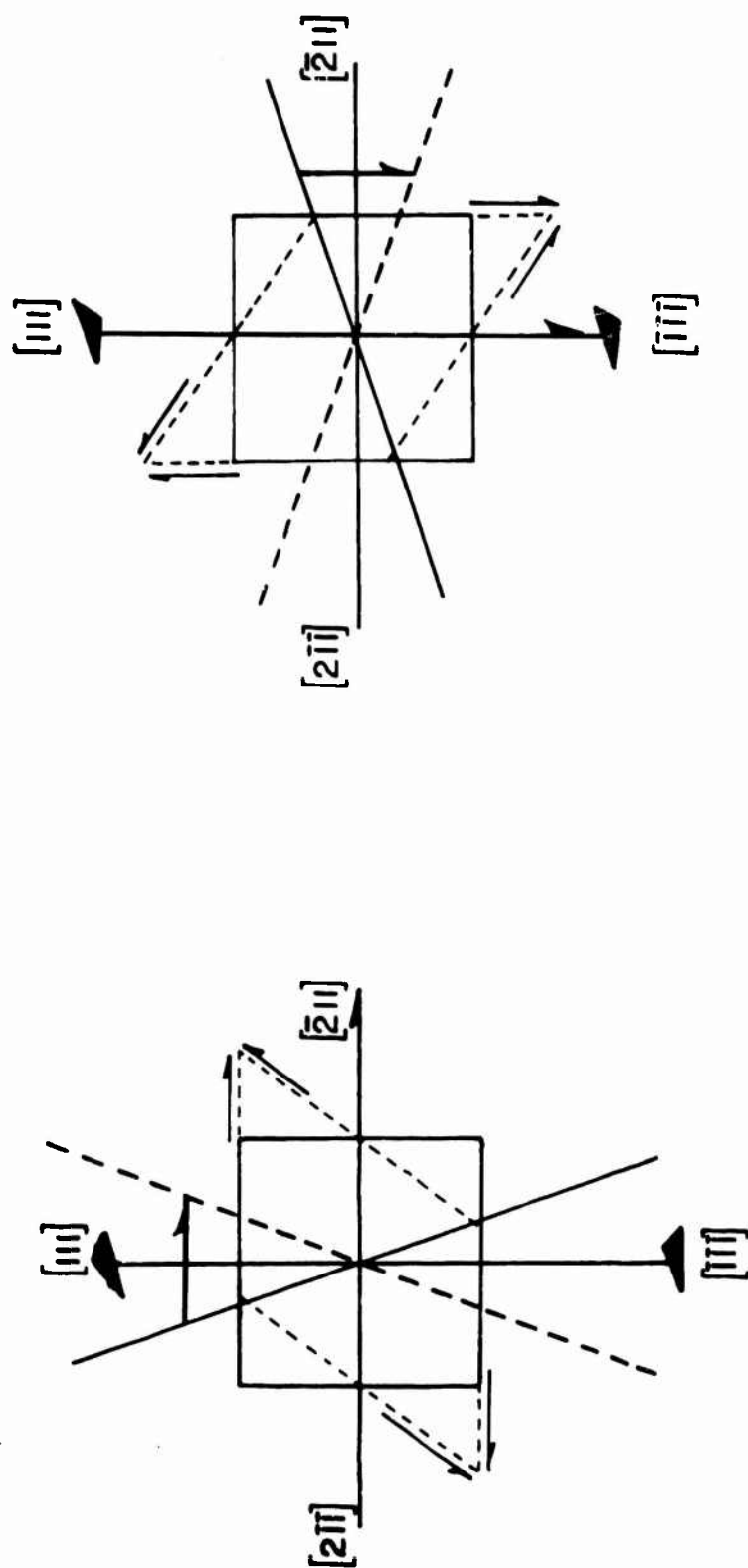
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Figure 4. Twin elements and shear deformation in twinning.

Following further the procedure of Frank and Thompson[5], it would be possible to draw additional sub-regions within which the set of possible systems is given an order of preference as a function of the magnitude of the resolved shear stress factor. Such diagrams are somewhat misleading, however, because experimental results tend to indicate that, regardless of the validity of the critical resolved shear stress criterion for twinning, in general only a limited number of twin systems will activate, and where multiple systems occur they will be those which are equally stressed or very nearly so. Accordingly, the systems of primary interest are those which have the largest Schmid factors. At high-symmetry orientations, multiple systems will be equally favored, and experimentally multiple twinning has been observed for such orientations,[1,6] at least under rapid impact conditions. Away from symmetry boundaries it would be assumed that secondary systems would not be activated, since the resolved shear stresses would be much lower. In the case of impact loading, however, it is known that very high stresses may be sustained for short periods. Thus, it is of interest to note that for certain orientations, the resolved shear stress on at least one secondary system is very nearly as high as that on the primary. Figures 5a and 5b were plotted from the output of the computer calculation for Schmid factors. The shaded areas indicate regions where the ratio of the Schmid factor on one or more secondary systems to the Schmid factor on the primary system exceeds 0.950. The boundary of this region for ratios exceeding 0.900 is indicated by the dotted line. In the fcc tension-bcc compression case, these regions are very narrow strips close to the symmetry lines, but in the frc compression-bcc tension case they cover a substantial portion of the standard triangle. It should be remembered that in this calculation the stress is assumed to be uniaxial, whereas in many real cases, including rapid impact loading, triaxial stresses undoubtedly exist and the actual resolved shear stresses would be different; however, despite the oversimplification of the uniaxial stress assumption, it might reasonably be expected that if very high stresses are applied in times of the order of
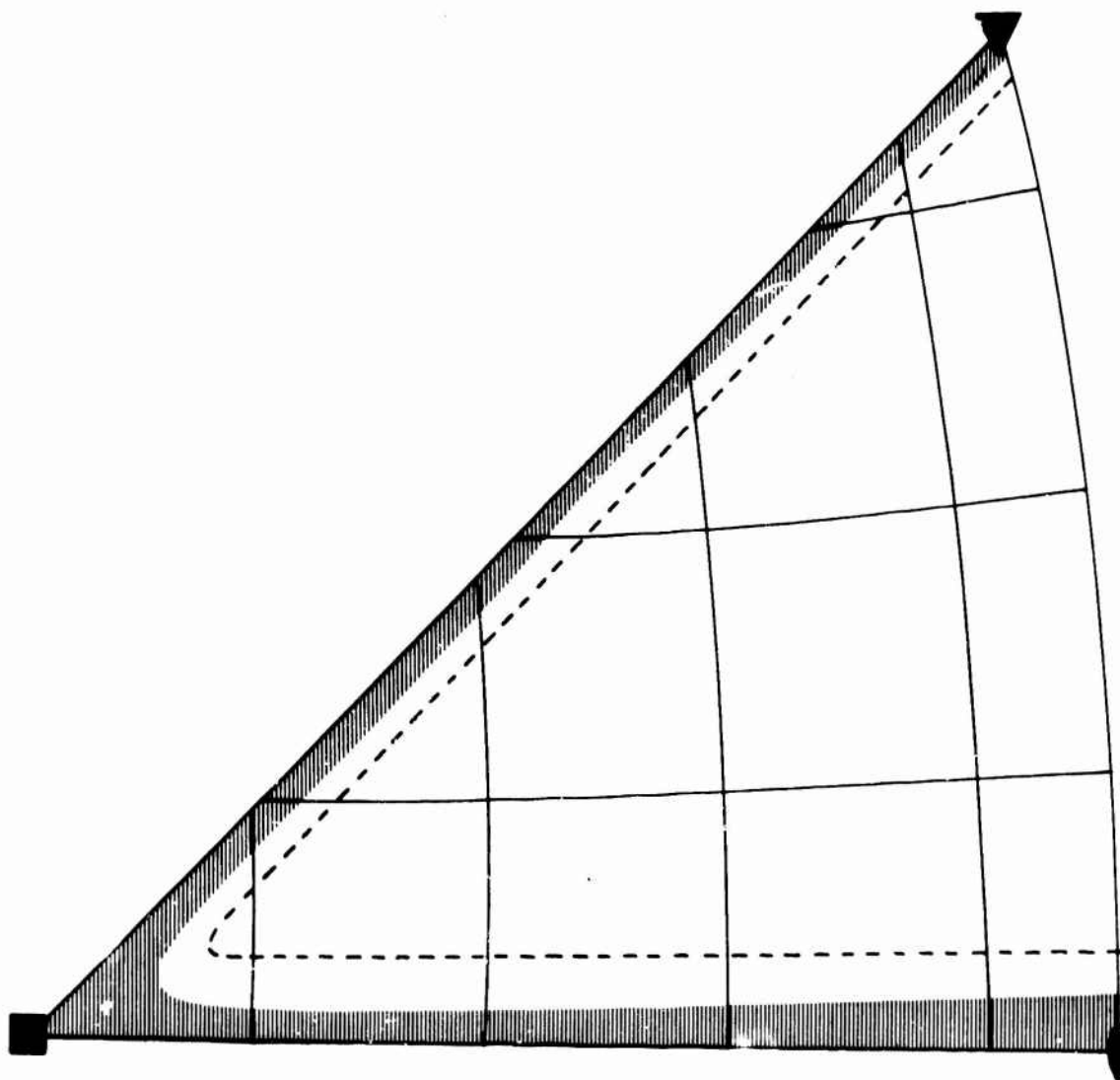
Figure 5a. Regions where the resolved shear stress on one or more secondary twin systems approaches the resolved shear stress on the primary, fcc tension and bcc compression.
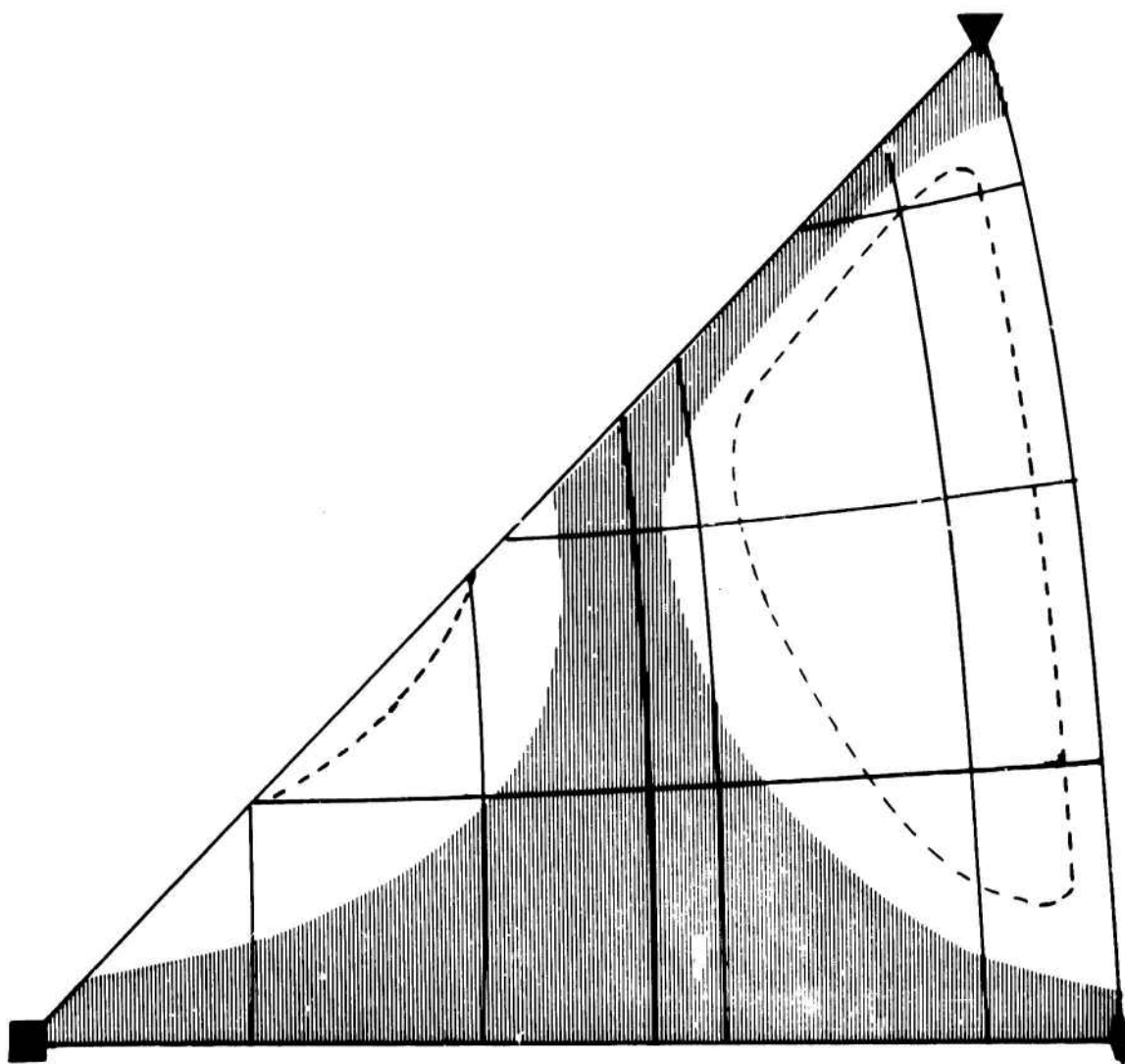
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Figure 5b. Regions where the resolved shear stress on one or more secondary twin systems approaches the resolved shear stress on the primary, fcc compression and bcc tension.

magnitude of those required for twinning to be initiated, or if complex stresses are present, the tension and compression behaviors of a given orientation in this region might be considerably different.

SUMMARY

A complete description of the resolved shearing stresses on the crystallographically equivalent {111} <$\bar{2}$11> fcc twinning modes and on the {$\bar{2}$11} <$\bar{1}\bar{1}$1> bcc twinning modes has been presented. The requirements for specifying twinning systems and the advantages of a systematic convention have been discussed.

Additional data have been included on the resolved shear stress factors as a function of orientation.

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DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY *(Corporate author)*	2a. REPORT SECURITY CLASSIFICATION
U. S. Army Aberdeen Research and Development Center Ballistic Research Laboratories Aberdeen Proving Ground, Maryland	Unclassified
	2b. GROUP

3. REPORT TITLE

RESOLUTION OF STRESSES IN DEFORMATION TWINNING

4. DESCRIPTIVE NOTES *(Type of report and inclusive dates)*

5. AUTHOR(S) *(First name, middle initial, last name)*

Priscilla W. Kingman

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
April 1969	29	6
8a. CONTRACT OR GRANT NO.	9a. ORIGINATOR'S REPORT NUMBER(S)	
b. PROJECT NO. RDT&E 1T061102A33E	Report No. 1433	
c.	9b. OTHER REPORT NO(S) *(Any other numbers that may be assigned this report)*	
d.		

10. DISTRIBUTION STATEMENT

This document has been approved for public release and sale; its distribution is unlimited.

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY
	U. S. Army Materiel Command Washington, D. C.

13. ABSTRACT

Solutions for the maximum resolved shear stresses on twinning systems in fcc and bcc crystals in tension and compression are presented and discussed. Additional data are included on the relative magnitudes of shear stresses on secondary systems. Conventions for the specification of twinning systems are described and discussed.

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Deformation Twins Crystallography Schmid Factor						